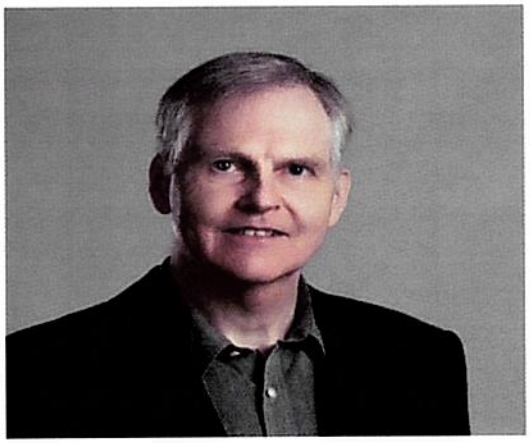
Quantum Brownian Motion: Facts, debatable issues and unsolved issues

Peter Hänggi and Gert Ingold

FQMT 2026, Prague,

26.July-01.August



where β is the coefficient of sliding friction if there is slip between the diffusing molecule and the solution. For N molecules of solute per c.c. of solution the total resistance will be N times this, and in the steady state of diffusion will equilibrate the driving force due to variation of the osmotic pressure of the solute, namely dp/dx, which by the osmotic laws is $RT\,dc/dx$, if c is the concentration of the solute at x and R is the gas constant. Hence

$$RT\frac{dc}{dx} = 6\pi V\eta a N\frac{1+2\eta/\beta a}{1+3\eta/\beta a}; \quad \ldots \quad (2)$$

and the required formula for the coefficient of diffusion with C for the number of molecules in a gramme-molecule is

$$D = \frac{RT}{6\pi\eta a C}\frac{1+3\eta/\beta a}{1+2\eta/\beta a} \quad \ldots \quad (3)$$

If $\beta=\infty$, that is, if there is no slipping of solution at surface of molecule, aD is the same for all molecules diffusing through a given solvent at a given temperature. Now for a large molecule of solute moving amongst smaller ones of solvent, we can see that the slipping is probably small. But in the other extreme case of a small molecule of solute moving amongst larger ones of solvent, an effect analogous to slipping will occur, since the small molecule will travel a good deal in the gaps which would be left if the molecules of solvent were forced almost into permanent contact. We have thus two extreme cases of the formula.

$$\left.\begin{aligned} &\text{When } \beta=0, \quad D=\frac{RT}{4\pi\eta a C}\\ &\text{and when } \beta=\infty, \quad D=\frac{RT}{6\pi\eta a C}\end{aligned}\right\} \quad \ldots \quad (4)$$

Thus with increasing values of a we should have aD diminishing from the upper limit $RT/4\pi\eta C$, when a is small, to the lower limit $RT/6\pi\eta C$, when a is large. This is analogous to the actual behaviour of B/D obtained from experiment, B being the volume of the molecules in a gramme-molecule of solute. The first of the following tables contains the coefficients of diffusion for various gases through water determined by Hüfner*. I have reduced these all to a temperature of 16° C., and expressed them with the second as unit of time instead of the day. The values of B are taken mostly from "Further Studies on Molecular Force" (Phil. Mag. [6] xxxix.). In the second last row are given the values of

* Wied. *Ann.* 1897, vol. xl., and *Zeit. f. Phys. Chem.* xxvii.

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Is quantum mechanics equivalent to a classical stochastic process?

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(Received 8 December 1978)

The authors analyze the connection between the theory of stochastic processes and quantum mechanics. It is shown that quantum mechanics is not equivalent to a Markovian diffusion process as claimed in recent papers. The origin of a possible confusion about this question is clarified. The authors further demonstrate that there does not even exist a non-Markovian process equivalent to quantum mechanics.

QUANTUM DISSIPATION

$$\mathcal{L} = \frac{1}{2} m_0 e^{\gamma t} \dot{x}^2 - \frac{1}{2} m_0 e^{\gamma t} \omega_0^2 x^2$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} = \frac{d}{dt} m_0 e^{\gamma t} \dot{x} = m_0 e^{\gamma t} \ddot{x} + m_0 e^{\gamma t} \gamma \dot{x}$$

$$-\frac{\partial \mathcal{L}}{\partial x} = m_0 e^{\gamma t} \omega_0^2 x$$

$$\Rightarrow \cancel{e^{\gamma t}} \left[m_0 \ddot{x} + m_0 \gamma \dot{x} + m_0 \omega_0^2 x \right] = 0$$

$$\text{QM: } \mathcal{L} \to H = \frac{p^2}{2m_0} e^{-\gamma t} + \frac{1}{2} m_0 e^{\gamma t} \omega_0^2 x^2$$

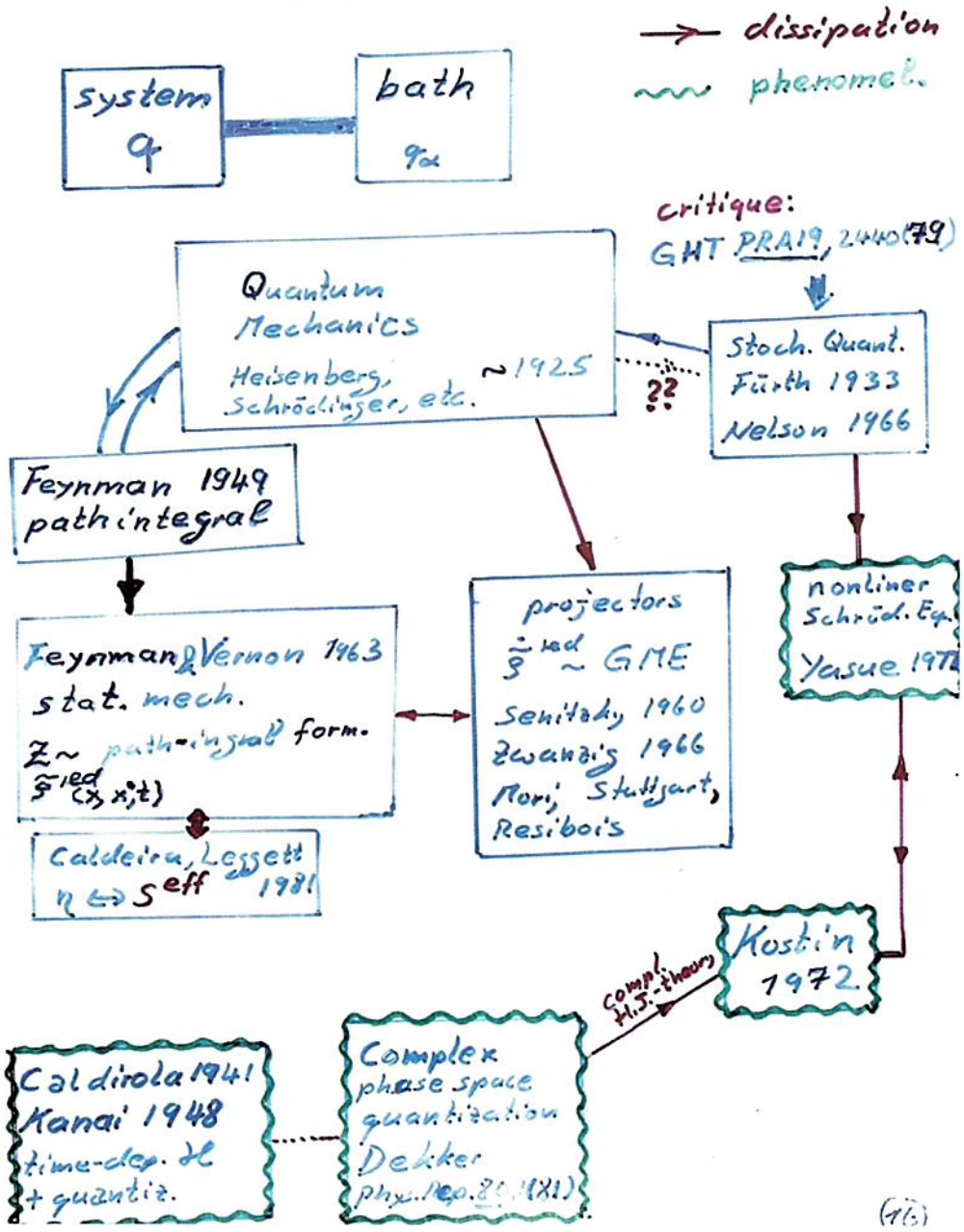
$$[\Delta x, \Delta p] = i\hbar e^{-\gamma t}$$

W. E. Brittin, Phys. Rev. 77, 396 (1950)

Chung-In Um, K. H. Yeon, T. F. George, Phys. Rep. 362, 63ff (2002) (129 pages!)

Quantum Dissipation

How ??



Quantum Semiclass. Opt. 8 (1996) 205–222. Printed in the UK

Quantum trajectories and quantum measurement theory

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Abstract. Beyond their use as numerical tools, quantum trajectories can be ascribed a degree of reality in terms of quantum measurement theory. In fact, they arise naturally from considering continuous observation of a damped quantum system. A particularly useful form of quantum trajectories is as linear (but non-unitary) stochastic Schrödinger equations. In the limit where a strong local oscillator is used in the detection, and where the system is not driven, these quantum trajectories can be solved. This gives an alternative derivation of the probability distributions for completed homodyne and heterodyne detection schemes. It also allows the previously intractable problem of real-time adaptive measurements to be treated. The results for an analytically soluble example of adaptive phase measurements are presented, and future developments discussed.

1. Introduction

The concept of stochastic Schrödinger equations (SSEs) [1] or quantum trajectories [2] has generated an impressive degree of activity in the quantum optics community over the past few years‡. To one outside the field, it may be hard to synthesize all of this activity, not least because there are (in my mind) three distinct interpretations of quantum trajectories. Here I am classifying authors by the ontological status which they ascribe to their quantum trajectories: not real; subjectively real; or objectively real. Alternatively, these three interpretations could be stated as quantum trajectories being, respectively, a mathematical tool; an application of quantum measurement theory; or a theory of microscopic state reduction. In the bulk of this paper I am concerned with quantum trajectories as a part of quantum measurement theory (that is, with what I am calling the subjective interpretation of quantum trajectories). Note that by 'measurement theory' I mean the body of mathematical techniques used to describe the process of measurement within the standard Copenhagen interpretation [3, 4] of quantum mechanics. I am not concerned with metaphysical arguments regarding the adequacy of the Copenhagen viewpoint, nor with physical extensions to standard quantum theory. However, interpretational issues have been raised in the context of quantum trajectories, and the potential confusion regarding the reality of SSEs may obscure the results I wish to present. For these reasons, I will begin with a brief review of the interpretations of quantum trajectories. I am not aware of a comparison of this sort being in print.

1.1. Non-real quantum trajectories

The 'non-real' interpretation of quantum trajectories treats the trajectories simply as numerical tools for solving the master equation. This is essentially the attitude taken by

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‡ Related ideas have also been developed by workers outside quantum optics. Space limitations prevent me from discussing these.

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Book H. M. Wiseman & G. J. Milburn
Quantum Measurement & Control
Cambridge Univ. Press 2010

real world quantum dissipation

- do not rely ("trust") more or less inspired guesswork
- do the full Q.M. in the universe

  do the hard work for a realistic Laboratory set-up ; - account for noise!

  Caldeira & Leggett, Grabert, Weiss, Hänggi, Schmid, Larkin, ...
- extract the relevant information by integration over bath degrees of freedom

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QUANTUM BROWNIAN MOTION: THE FUNCTIONAL INTEGRAL APPROACH

Hermann GRABERT, Peter SCHRAMM and Gert-Ludwig INGOLD

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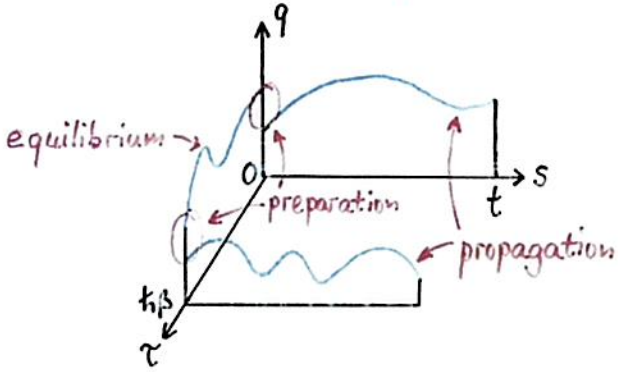
NORTH-HOLLAND · AMSTERDAM

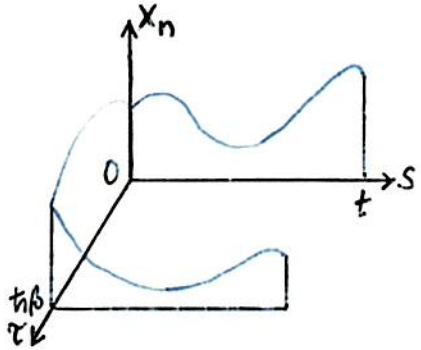
density matrix of system + heat bath:

$$W(t) = e^{-\frac{i}{\hbar}Ht} \sum_j (O_j\, e^{-\beta H} O_j')\, e^{\frac{i}{\hbar}Ht}$$

use functional integrals



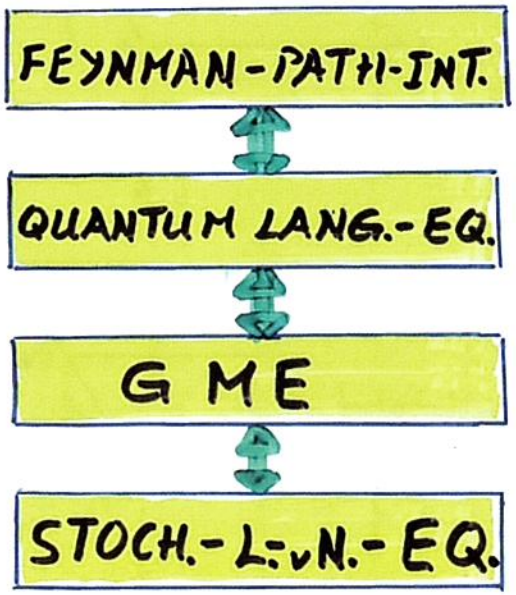
system



heat bath

QUANTUM NOISE

NO QUANTUM EQ.-PARTITION-TH.



$$s := |\psi_1(t)\rangle\langle\psi_2(t)| \;,\; \mu := \frac{2}{\pi}\int_0^\infty d\omega\, \frac{J(\omega)}{\omega}$$

$$i\hbar\dot{s} = [H_0, s] + \frac{\mu}{2}[x^2, s] - \xi(t)[x, s] - \frac{\hbar}{2}\nu(t)\{x, s\}_+$$

COMPLEX VALUED NOISE

$$\langle \xi(t)\xi(t')\rangle = \mathrm{Re}\,L(t-t')\,;\quad \langle \xi(t)\nu(t')\rangle = \frac{2i}{\hbar}\theta(t-t')\,\mathrm{Im}\,L(t-t')$$
$$\langle \nu(t)\nu(t')\rangle = 0$$

PHYSICAL REVIEW A **69**, 052109 (2004)

Is the dynamics of open quantum systems always linear?

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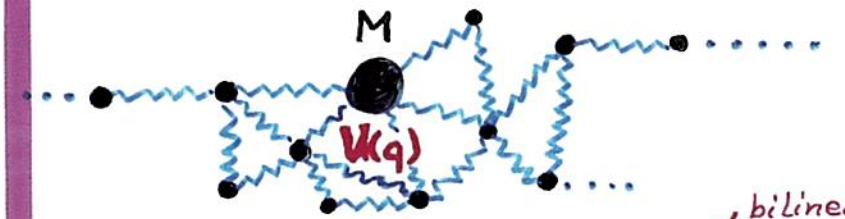
(Received 1 December 2003; published 17 May 2004)

We study the influence of the preparation of an open quantum system on its reduced time evolution. In contrast to the frequently considered case of an initial preparation where the total density matrix factorizes into a product of a system density matrix and a bath density matrix the time evolution generally is no longer governed by a linear map nor is this map affine. Put differently, the evolution is truly nonlinear and cannot be cast into the form of a linear map plus a term that is independent of the initial density matrix of the open quantum system. As a consequence, the inhomogeneity that emerges in formally exact generalized master equations is in fact a nonlinear term that vanishes for a factorizing initial state. The general results are elucidated with the example of two interacting spins prepared at thermal equilibrium with one spin subjected to an external field. The second spin represents the environment. The field allows the preparation of mixed density matrices of the first spin that can be represented as a convex combination of two limiting pure states, i.e., the preparable reduced density matrices make up a convex set. Moreover, the map from these reduced density matrices onto the corresponding density matrices of the total system is affine only for vanishing coupling between the spins. In general, the set of the accessible total density matrices is nonconvex.

dissipation



$$H^T = H_{system} + H_{bath} + H_{Int}$$

(bilinear)

$$\ddot{q} = -\frac{1}{M}\frac{\partial U}{\partial q} - \int_0^t \gamma(t-s)\,\dot{q}(s)\,ds$$

$$S_E = S_{\text{rev. motion}} + S_{\substack{\text{(nonlocal)}\\ \text{dissipation}}}$$

microscopic approach

$$H^{total} = \underbrace{\frac{1}{2} M \dot{q}^2 + U(q)}_{\text{system}}$$

$$+ \underbrace{\frac{1}{2} \sum_\alpha m_\alpha \dot{q}_\alpha^2 + \sum_\alpha m_\alpha \omega_\alpha^2 q_\alpha^2}_{\text{(harmonic) bath}}$$

$$+ \underbrace{q \sum_\alpha c_\alpha q_\alpha}_{\text{linear coupling}}$$

$$+ \underbrace{q^2 \sum_\alpha \frac{c_\alpha^2}{2 m_\alpha \omega_\alpha^2}}_{\text{compensation of frequency shift}}$$

- path integral approach to density matrix at temperature T
- trace out environment

See in: [redacted]

P. H. & G. Ingold

Q L E

Chaos 15, 026105 (2005)

$$i\hbar\dot{O} = [O, H_T]$$

$$m\ddot{x} + m\int_0^t ds\, \gamma(t-s)\dot{x}(s) + \frac{\partial V(x)}{\partial x} = \eta(t) - m\gamma(t-0)x(0)$$

INITIAL SLIP

$$! \quad \gamma(t-s) = \frac{1}{m}\sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha^2}\cos(\omega_\alpha(t-s))$$

$$= \gamma(s-t)$$

$$\eta(t) = \sum_\alpha c_\alpha \left[q_\alpha(0)\cos(\omega_\alpha t) + \frac{p_\alpha}{m_\alpha\omega_\alpha}\sin(\omega_\alpha t)\right]$$

- $[\eta(t), \eta(s)] = -i\hbar \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \sin(\omega_\alpha (t-s))$

$\neq 0$

$\rho_B = Z^{-1} \exp\left\{-\beta\left[\sum_\alpha \left(\frac{1}{2}\frac{p_\alpha^2}{m_\alpha} + \frac{m\omega_\alpha^2}{2} q_\alpha^2\right)\right]\right\}$

- $\langle \eta(t) \rangle_{\rho_B} = 0$

- $\frac{1}{2}\langle \eta(t)\eta(s) + \eta(s)\eta(t) \rangle = C(t-s)$

$= C(\tau) = \frac{\hbar}{2} \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \coth\left(\frac{\hbar\omega_\alpha}{2kT}\right) \cos(\omega_\alpha \tau)$

$kT \gg \hbar\omega_\alpha$ ⟶ $kT\,\gamma(\tau)$

REMARKS

1.

QLE OPERATES IN FULL HILBERT SPACE OF S⊕B

2

$$\hat{\chi}(z) = \int_0^\infty e^{izt}\, \chi(t)\, dt = \frac{i}{2m} \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha^2} \left[\frac{1}{z - \omega_\alpha} + \frac{1}{z + \omega_\alpha} \right]$$

$$\frac{1}{x + i0^+} = P\left(\frac{1}{x}\right) - i\pi\delta(x) \qquad \mathrm{Im}\, z > 0$$

$$\mathrm{Re}\,\hat{\chi}(z = \omega + i0^+) = \frac{\pi}{2m} \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha^2} \left[\delta(\omega - \omega_\alpha) + \delta(\omega + \omega_\alpha) \right]$$

$$\rightarrow \boxed{C(\tau) = \frac{m}{\pi} \int_0^\infty d\omega\, \mathrm{Re}\,\hat{\chi}(\omega + i0^+)\, \cos(\omega\tau) \cdot \coth\left(\frac{\hbar\omega}{2kT}\right)}$$

3 with $\hat{\xi}(t) = m\ddot{\eta}(t) - m\gamma(t) * \eta(0)$

$$\hat{\rho}_B = Z^{-1} \exp -\beta \left[\sum_\alpha \left(\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} \left(q_\alpha - \frac{c_\alpha}{m_\alpha \omega_\alpha^2} x \right)^2 \right) \right]$$

$$\rightarrow \langle \hat{\xi}(t) \rangle_{\hat{\rho}_B} = 0$$

$$\Rightarrow \langle \hat{\xi}(\tau)\hat{\xi}(0) + \hat{\xi}(0)\hat{\xi}(t) \rangle_{\hat{\rho}_B} = C(\tau)$$

PITFALLS

MARKOV MASTER EQ

$$\frac{d}{dt}\rho = -\frac{i}{\hbar} L\rho - \Gamma\rho + I(t)$$

BLOCH-REDFIELD

i.g. NO DET. BALANCE

ROTATING WAVE APPROX.

(LINDBLAD; DAVIES-APPROX.)

DET. BALANCE ✓ O.K.

BUT

- WRONG EHRENFEST EQ.
- NO FDT
- NO KMS-COND. $\langle u(t)\, v\rangle_\beta = \langle v\, u(t+i\hbar\beta)\rangle_\beta$

4. ⚠ DEPHASING AT T = 0 !

$$\langle x(0)\xi(t)\rangle_{\hat{\xi}} \neq 0$$

$$\langle H_{INT}\rangle_{\hat{\xi}} \neq 0$$

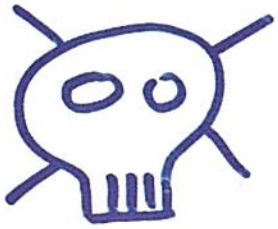
5.

$\xi(t) \longrightarrow$ C-NOISE $\xi(t)$

WITH CORRELATION

$C(\tau)$

IS INCONSISTENT



TIME REVERSAL

$$m\ddot{x} + m\int_0^t ds\, \gamma(t-s)\dot{x}(s) + \frac{\partial V}{\partial x} = -m\gamma(t)x(0) + \xi(t)$$

$$y(0) = x(0)$$
$$q_\alpha(0) = q_\alpha(0)$$
$$p_\alpha(0) = -p_\alpha(0)$$

$t \to -t \Rightarrow y = x(-t)$

WITH $\dot{y}(t) = \frac{d}{dt}x(-t) = -\dot{x}(-t)$

$$\dot{y}(t) = \ddot{x}(-t)$$
$$\dot{x}(s) = -\dot{y}(-s)$$

$$m\ddot{y}(t) + m\int_0^{-t} ds\, \gamma(-s-t)[-\dot{y}(-s)] + \frac{\partial V}{\partial y} = -m\gamma(t)x(0) + \xi(t)$$

$\tau = -s \; ; \; ds = -d\tau$

$\gamma(\tau - t) = \gamma(t - \tau)$

$$\Rightarrow m\ddot{y}(t) + m\int_0^t d\tau\, \gamma(t-\tau)\dot{y}(\tau) + \frac{\partial V}{\partial y} = -m\gamma(t)y(0) + \xi(t)$$

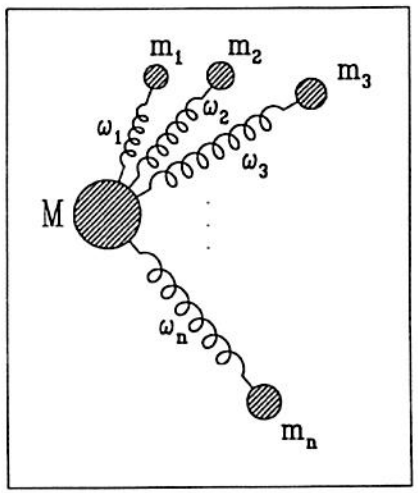
OHMIC FRICTION: $\gamma(t-s) = 2\gamma\delta(t-s)$

$$m\ddot{x} = -\frac{\partial V}{\partial x} - m\gamma\dot{x}\begin{cases} 1; & t>0 \\ -1; & t<0 \end{cases} + \xi(t)$$

FREE QUANTUM Brownian MOTION

Using the path integral methodology in full phase space of system + bath + interaction

free Brownian Quantum motion



$$U(q) = 0$$

$$c_n = m_n \omega_n^2$$

$$H = \frac{p^2}{2M_0} + \sum_{n=1}^{N\to\infty} \left[\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 (q_n - q)^2 \right]$$

translationally invariant

displacement correlation fct.

$$Q^{F}(t) = \frac{1}{2}\left\{ \langle [q(t)-q(0)]\, q(0)\rangle + \langle q(0)[q(t)-q(0)]\rangle \right\}$$

$$= \frac{1}{2}\left\{ \langle q(t)q(0)\rangle - \langle q^2(0)\rangle + \langle q(0)q(t)\rangle - \langle q^2(0)\rangle \right\}$$

$$= \underbrace{\frac{1}{2}\left\{ \langle q(t)q(0)\rangle + \langle q(0)q(t)\rangle \right\}}_{S(t)} - \langle q^2(0)\rangle$$

$S(t)$ ← diverges! for $\omega_0 \to 0$ $\propto k_B T/M\omega_0$

$$= \underbrace{S(t) - \langle q^2\rangle_{eq}}_{\text{is regular}}$$

mean square displacement: $s(t)$

$$s(t) = \langle (q(t)-q(0))^2 \rangle = \langle (q(t)-q(0))(q(t)-q(0)) \rangle$$

$$= \langle q^2(t)\rangle + \langle q^2(0)\rangle - \langle q(t)q(0)\rangle - \langle q(0)q(t)\rangle$$

$$\boxed{s(t) = -2\,Q^{F}(t)} + \underbrace{\langle q^2(t)\rangle_{eq} + \langle q^2(0)\rangle_{eq} - 2\langle q^2(0)\rangle_{eq}}_{0}$$

at $T=0$ $\quad s(t) \xrightarrow{T\to 0} \equiv s_0(t)$ notation

Table 3

Asymptotic long-time dependence of the mean square displacement [$s_0(t)$ for $T=0$ and $s(t)$ for $T>0$] and the antisymmetrized part $A^F(t)$ of the displacement correlation function in terms of the exponent α and the quantities defined in eqs. (11.19–11.23). The symmetrized part $Q^F(t)$ of the displacement correlation function is given by $Q^F(t) = -s(t)/2$

α	$s_0(t)$ $[T=0]$	$A^F(t)$	$s(t)$ $[T>0]$
$0<\alpha<1$	$2q_\infty$	$-(\alpha\hbar/2\mu_\alpha)t^{\alpha-1}$ $\times[1+O(t^{-1}, t^{\alpha-2})]$	$2D_\alpha t^\alpha$ $\times[1+O(t^{-1}, t^{\alpha-2})]$
$\alpha=1$	$2d_1 \ln(t)$ $\times[1+O(\ln^{-1}(t))]$		
$1<\alpha<2$	$2d_\alpha t^{\alpha-1}$ $\times[1+O(t^{\alpha-2})]$		
$\alpha=2$	$2d_2 t/\ln^2(t)$ $\times[1+O(\ln^{-1}(t))]$	$-(\hbar/\mu_2)t/\ln(t)$ $\times[1+O(\ln^{-1}(t))]$	$2D_2 t^2/\ln(t)$ $\times[1+O(\ln^{-1}(t))]$
$2<\alpha<3$	$2d_\alpha t^{3-\alpha}$ $\times[1+O(t^{2-\alpha})]$	$-(\hbar/2M_r)t$ $\times[1+O(t^{-2}, t^{2-\alpha})]$	$2(v_\beta^2/2)t^2$ $\times[1+O(t^{-2}, t^{2-\alpha})]$
$\alpha=3$	$2d_3 \ln(t)$ $\times[1+O(\ln^{-1}(t))]$		
$3<\alpha$	constant		

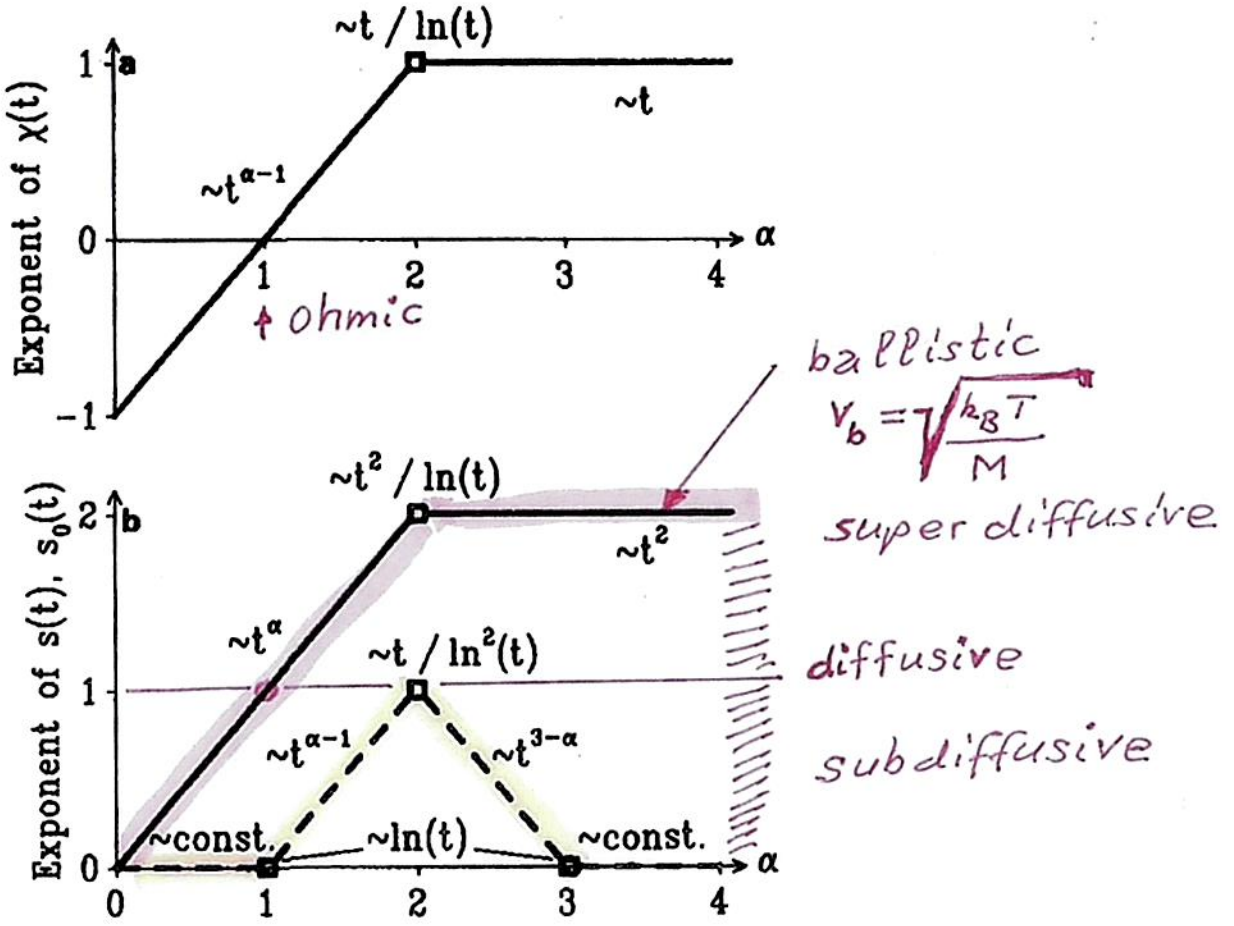


Fig. 7. (a) The exponent of the asymptotic time dependence of the response function $\chi(t)$ is shown as a function of the spectral exponent α. (b) The solid (dashed) line shows the exponent of the asymptotic time dependence of the mean square displacement $s(t)(s_0(t))$ for finite (zero) temperature as a function of the spectral exponent α.

Quantum Brownian motion and the Third Law of thermodynamics

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Acta Phys. Pol. B **37**, 1537 (2006)
New J. Phys. **10**, 115008 (2008)
Phys. Rev. E **79**, 061105 (2009)
J. Phys. A (Fast Track) **42**, 392002 (2009)

Model for a damped free particle

Hamiltonian

$$H = H_S + H_B + H_{SB}$$

$$= \frac{p^2}{2M} + \sum_{n=1}^{\infty}\left(\frac{p_n^2}{2m_n} + \frac{m_n}{2}\omega_n^2 x_n^2\right) + \sum_{n=1}^{\infty}\left(-c_n x_n q + \frac{c_n^2}{2m_n\omega_n^2} q^2\right)$$

translational invariance: $c_n = m_n\omega_n^2$

$$= \frac{p^2}{2M} + \sum_{n=1}^{\infty}\left(\frac{p_n^2}{2m_n} + \frac{m_n}{2}\omega_n^2 (x_n - q)^2\right)$$

Quantum Langevin equation

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}q + M\int_{t_0}^{t}\mathrm{d}s\gamma(t-s)\frac{\mathrm{d}}{\mathrm{d}s}q = \xi(t)$$

▸ damping kernel and noise

Drude model

damping kernel

$$\gamma(t) = \gamma\omega_{\mathrm{D}} \mathrm{e}^{-\omega_{\mathrm{D}} t}$$

Quantum Langevin equation

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}q + M\gamma\omega_{\mathrm{D}}\int_{t_0}^{t}\mathrm{d}s\,\mathrm{e}^{-\omega_{\mathrm{D}}(t-s)}\frac{\mathrm{d}}{\mathrm{d}s}q = \xi(t)$$

equivalent equations of motion

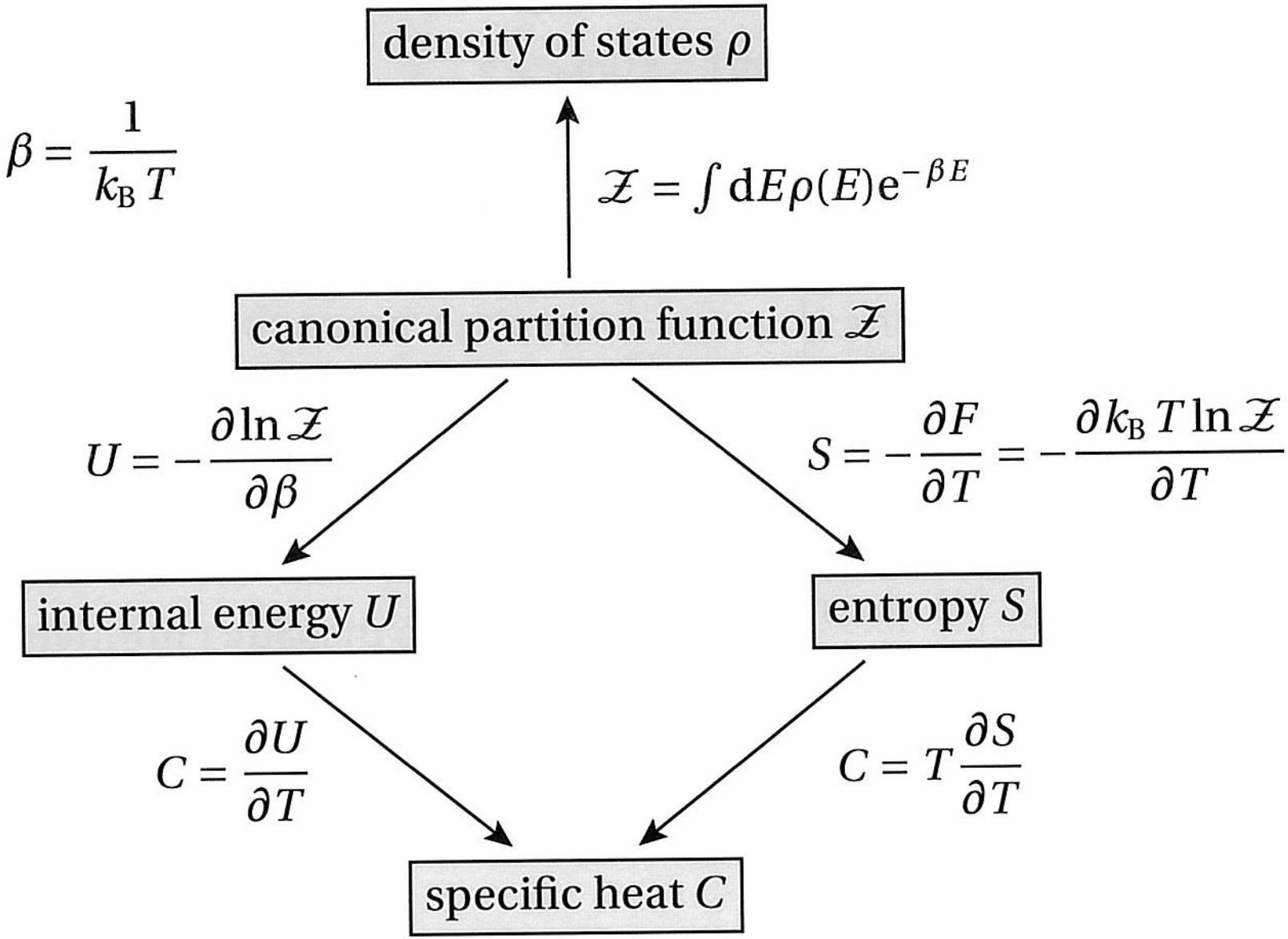
$$\dot{q} = v$$

$$\dot{v} = z$$

$$\dot{z} = -\omega_{\mathrm{D}} z - \gamma\omega_{\mathrm{D}} v$$

oscillations occur for $\omega_{\mathrm{D}} < 4\gamma$

A bit of thermodynamics



Free energy of a system strongly coupled to an environment

Thermodynamic argument:

$$\mathcal{Z} = \frac{\mathrm{Tr}_{\mathrm{S+B}}(\mathrm{e}^{-\beta H})}{\mathrm{Tr}_{\mathrm{B}}(\mathrm{e}^{-\beta H_{\mathrm{B}}})} \qquad \longrightarrow \qquad F_{\mathrm{S}} = F - F_{\mathrm{B}}^{0}$$

F total system free energy

F_{B} bare bath free energy

With this form of free energy the three laws of thermodynamics are fulfilled.

P. Hänggi, G.-L. Ingold, P. Talkner, New J. Phys. **10**, 115008 (2008)

G.-L. Ingold, P. Hänggi, P. Talkner, Phys. Rev. E **79**, 061105 (2009)

An important difference

Route I

$$E \doteq E_S = \langle H_S \rangle = \frac{\mathrm{Tr}_{S+B}(H_S e^{-\beta H})}{\mathrm{Tr}_{S+B}(e^{-\beta H})}$$

Route II

$$\mathcal{Z} = \frac{\mathrm{Tr}_{S+B}(e^{-\beta H})}{\mathrm{Tr}_B(e^{-\beta H_B})} \qquad U = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}$$

$$\Rightarrow U = \langle H \rangle - \langle H_B \rangle_B$$

$$= E_S + \left[\langle H_{SB} \rangle + \boxed{\langle H_B \rangle - \langle H_B \rangle_B} \right]$$

For finite coupling E and U differ!

Partition function and internal energy

undamped case

$$Z_0 = \frac{L}{\hbar}\left(\frac{2\pi m}{\beta}\right)^{1/2}$$

with damping

$$Z = Z_0 \prod_{n=1}^{\infty} \frac{\nu_n}{\nu_n + \hat{\gamma}(\nu_n)}$$

internal energy ▸ compare with energy E

$$U = \frac{1}{2\beta}\left[1 + 2\sum_{n=1}^{\infty} \frac{\hat{\gamma}(\nu_n) - \nu_n \hat{\gamma}'(\nu_n)}{\nu_n + \hat{\gamma}(\nu_n)}\right]$$

$$= \frac{\hbar\omega_D}{2\pi}\psi\left(\frac{\hbar\beta\omega_D}{2\pi}\right) - \frac{x_+}{\beta}\psi(x_+) - \frac{x_-}{\beta}\psi(x_-) - \frac{1}{2\beta}$$

Specific heat from partition function

$$\frac{C^Z}{k_B} = x_1^2\psi'(x_1) + x_2^2\psi'(x_2) - \left(\frac{\hbar\beta\omega_D}{2\pi}\right)^2 \psi'\left(\frac{\hbar\beta\omega_D}{2\pi}\right) - \frac{1}{2}$$

with

$$x_{1,2} = \frac{\hbar\beta\omega_D}{4\pi}\left(1 \pm \sqrt{1 - \frac{4\gamma}{\omega_D}}\right)$$

high-temperature expansion

$$\frac{C^Z}{k_B} = \frac{1}{2} - \frac{\hbar^2\gamma\omega_D}{12(k_B T)^2} + O(T^{-3})$$

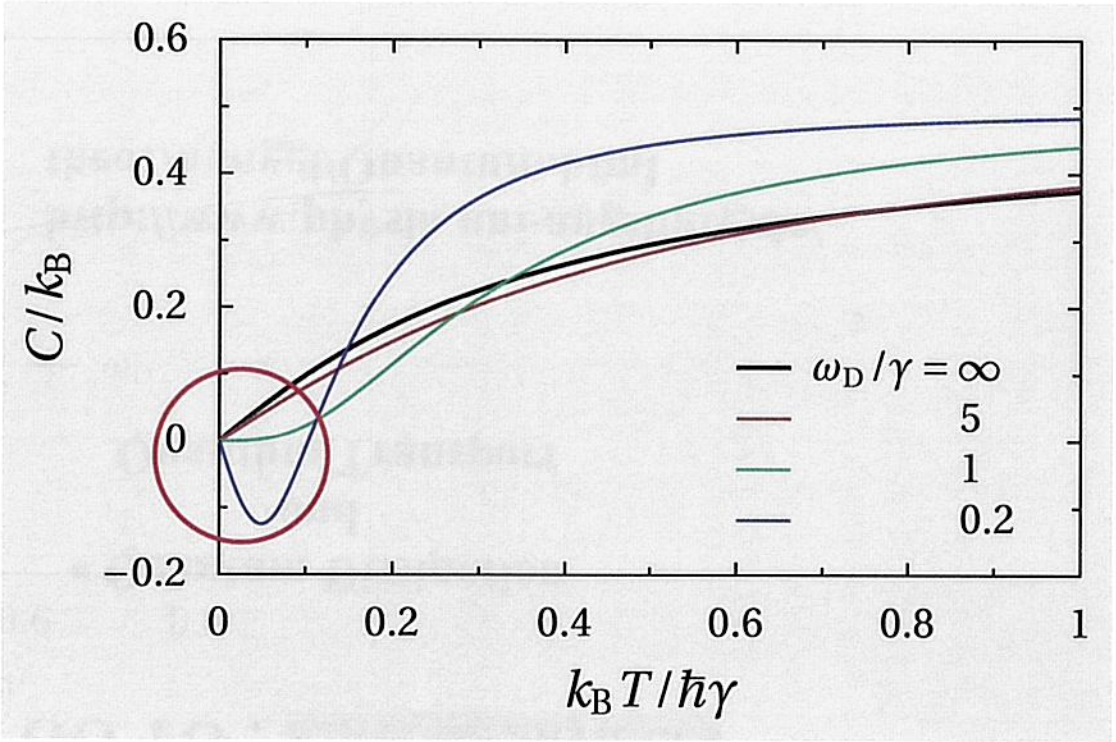
low-temperature expansion

$$\frac{C^Z}{k_B} = \frac{\pi}{3}\frac{k_B T}{\hbar\gamma}\left(1 - \frac{\gamma}{\omega_D}\right) - \frac{4\pi^3}{15}\left(\frac{k_B T}{\hbar\gamma}\right)^3\left[1 - 3\frac{\gamma}{\omega_D} - \left(\frac{\gamma}{\omega_D}\right)^3\right] + O(T^5)$$

return

Specific heat of a damped free particle

Universität Augsburg University



P. Hänggi, GLI, P. Talkner, New J. Phys. **10**, 115008 (2008)

damping kernel: $\gamma(t) = \gamma\omega_D e^{-\omega_D t}$

$$\hat{\gamma}(z) = \frac{\gamma\omega_D}{z+\omega_D}$$

HOMEPAGE
„HANGGI“

GO TO : FEATURE ARTICLES

- **Quantum Dissipation**
  and
  Quantum Transport

http://www.physik.uni-augsburg.de/theo1/hanggi/Quantum.html